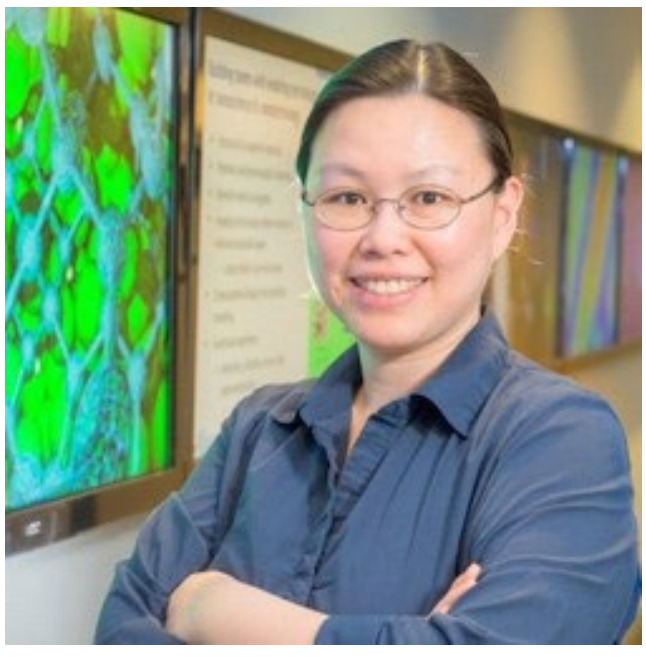
Department of Physics
Arizona State University

COLLOQUIUM



Refreshments at 3:45pm in PSF 186

Colloquium from 4:00 PM – 5:00 PM in PSF 101

Theory-informed AI/ML for Design and Characterization of Energy Materials

Dr. Maria Chan

Argonne National Lab

Abstract:

In materials and chemical science, the combination of high throughput computational modeling and experimentation has given rise to significant challenges and opportunities. Data science techniques such as machine learning, artificial intelligence, and computer vision have made a significant impact in the ease, scope, and speed of understanding of known materials and discovery of new ones. In this talk, we will discuss how we use data science approaches in conjunction with theory-based modeling to interpret experimental characterization data (such as x-ray scattering, spectroscopy, scanning probe microscopy, and electron microscopy) and carry out materials design (such as in the space of classic zinc blende and hybrid perovskite optoelectronic materials).

Biography:

Maria Chan obtained her BSc in Physics and Applied Mathematics from the University of California, Los Angeles, and PhD in Physics from the Massachusetts Institute of Technology. Since 2012, Dr. Chan has been a staff scientist at the Center of Nanoscale Materials, part of Argonne National Laboratory near Chicago. Dr. Chan's research focuses on the computational prediction of materials properties, using first principles, atomistic, and machine learning methods, particularly in applications towards materials relevant to energy technologies. She also works on the integration of experimental characterization and computational modeling using artificial intelligence and machine learning approaches. She has joint appointments at Northwestern University and the University of Chicago, and is an Associate Editor at ACS Chemistry of Materials.

Host: Prof. Arunima Singh

View our Fall 2022 Physics Colloquium schedule at https://physics.asu.edu/colloquia